

We claim:

1. A method for evaluating process conditions for a catalyzed chemical reaction in a parallel flow reactor, the method comprising

simultaneously supplying one or more reactants to each of six or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the six or more reactors comprising a catalyst having activity for the chemical reaction, each of the six or more catalysts having substantially the same composition,

controllably varying a set of reaction conditions between each of the six or more reactors, the varied set of reaction conditions comprising (i) at least three different space velocities or contact times or combinations thereof, and (ii) at least two different temperatures, pressures or feed compositions,

simultaneously discharging a reactor effluent from each of the six or more reactors, and

analyzing the reactor effluent from each of the six or more reactors to determine the conversion of one or more reactants and the selectivity for one or more products of the chemical reaction of interest in each of the reactors.

2. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of values that span at least about 10% conversion difference.

3. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of values that span at least about 20% conversion difference.

4. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of values that span at least about 40% conversion difference.

5. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 20% to more than about 40%.

6. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 10% to more than about 50%.

7. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 10 % to more than about 70 %.

8. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 2 % to more than about 5 %.

9. The method of claim 1 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 1 % to more than about 10%.

10. The method of claim 1 wherein the reactor effluent from each of the six or more reactors are simultaneously analyzed.

11. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different temperatures.

12. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different pressures.

13. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different feed compositions.

14. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different temperatures.

15. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different pressures.

16. The method of claim 1 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different feed compositions.

17. The method of claim 1 wherein  
one or more reactants are simultaneously supplied to each of twelve or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the twelve or more reactors comprising a catalyst having activity for the chemical reaction, each of the twelve or more catalysts having substantially the same composition,

a first set of reaction conditions is controllably varied between each of a first set of six or more reactors, the first set of reaction conditions comprising (i) at least three different space velocities, and (ii) at least two different temperatures, the method further comprising

controllably varying a second set of reaction conditions between each of a second set of six or more reactors, the second set of reaction conditions comprising (i) at least three different space velocities, and (ii) at least two different feed compositions.

18. The method of claims 1 or 17 wherein each of the catalysts are prepared under substantially the same conditions.

19. The method of claims 1 or 17 wherein each of the catalysts are substantially the same catalysts.

20. A method for evaluating process conditions for a catalyzed chemical reaction in a parallel flow reactor, the method comprising

simultaneously supplying one or more reactants to each of six or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the six or more reactors comprising a catalyst having activity for the chemical reaction, each of the six or more catalysts having substantially the same composition,

controllably varying a set of reaction conditions between each of the six or more reactors, the varied set of reaction conditions comprising (i) at least three different space velocities, and (ii) at least two different contact times,

simultaneously discharging a reactor effluent from each of the six or more reactors, and

analyzing the reactor effluent from each of the six or more reactors to determine the conversion of one or more reactants and the selectivity for one or more products of the chemical reaction of interest in each of the reactors.

21. The method of claim 20 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of values that span at least about 10% conversion difference.

22. The method of claim 20 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of values that span at least about 20% conversion difference.

23. The method of claim 20 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more

reactions includes a range of six values ranging from less than about 2 % to more than about 5 %.

24. The method of claim 20 wherein the set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 1 % to more than about 10 %.

25. The method of claim 20 wherein the set of reaction conditions are varied such that a determined conversion of the conversion-limiting reactant for the six or more reactions includes a range of six values ranging from less than about 20% to more than about 40%.

26. The method of claim 20 wherein the range of six values for the determined conversion ranges from about 10% to about 50%.

27. A method for evaluating process conditions for a catalyzed chemical reaction in a parallel flow reactor, the method comprising

simultaneously supplying one or more reactants to each of twelve or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the twelve or more reactors comprising a catalyst having activity for the chemical reaction, a first set of six or more of the catalysts having substantially the same first composition, a second set of six or more of the catalysts having substantially the same second composition, the second composition being different from the first composition,

controllably varying a first set of reaction conditions between each of the six or more reactors comprising the first set of catalysts, the varied first set of reaction conditions comprising (i) at least three different space velocities or contact times or combinations thereof, and (ii) at least two different temperatures, pressures or feed compositions,

controllably varying a second set of reaction conditions between each of the six or more reactors comprising the second set of catalysts, the varied second set of reaction conditions comprising (i) at least three different space velocities or contact times or

combinations thereof, and (ii) at least two different temperatures, pressures or feed compositions,

simultaneously discharging a reactor effluent from each of the twelve or more reactors, and

analyzing the reactor effluent from each of the twelve or more reactors to determine the conversion of one or more reactants and the selectivity for one or more products of the chemical reaction of interest in each of the reactors.

28. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of values that span at least about 10% conversion difference, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of values that span at least about 10% conversion difference.

29. The method of claim 27 wherein the first set of reaction conditions are varied such that determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of values that span at least about 20% conversion difference, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of values that span at least about 20% conversion difference.

30. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of values that span at least about 40% conversion difference, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of values that span at least about 40% conversion difference.

31. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 20% to more than about 40%, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 20% to more than about 40%.

32. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 10% to more than about 50%, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 10% to more than about 50%.

33. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 10% to more than about 70%, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 10 % to more than about 70%.

34. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 2 % to more than about 5 %, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 2 % to more than about 5 %.

35. The method of claim 27 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 1 % to more than about 10%, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 1 % to more than about 10%.

36. The method of claim 27 wherein the reactor effluent from each of the twelve or more reactors are simultaneously analyzed.

37. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different space velocities, and (ii) at least two different temperatures.

38. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different space velocities, and (ii) at least two different pressures.

39. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different space velocities, and (ii) at least two different feed compositions.

40. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different contact times, and (ii) at least two different temperatures.

41. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different contact times, and (ii) at least two different pressures.



42. The method of claim 27 wherein the varied first and second sets of reaction conditions each comprise (i) at least three different contact times, and (ii) at least two different feed compositions.

43. The method of claim 27 wherein each of the six or more catalysts of the first set of catalysts are prepared under substantially the same first set of preparation conditions, and each of the six or more catalysts of the second set of catalysts are prepared under substantially the same second set of preparation conditions, the first set and second set of preparation conditions being the same as or different from each other.

44. The method of claim 27 wherein each of the six or more catalysts of the first set of catalysts are substantially the same first catalysts, and each of the six or more catalysts of the second set of catalysts are substantially the same second catalysts.

45. A method for evaluating process conditions for a catalyzed chemical reaction in a parallel flow reactor, the method comprising

simultaneously supplying one or more reactants to each of twelve or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the twelve or more reactors comprising a catalyst having activity for the chemical reaction, a first set of six or more of the catalysts having substantially the same first composition, a second set of six or more of the catalysts having substantially the same second composition, the second composition being different from the first composition,

controllably varying a first set of reaction conditions between each of the six or more reactors comprising the first set of catalysts, the varied first set of reaction conditions comprising (i) at least three different space velocities, and (ii) at least two different contact times,

controllably varying a second set of reaction conditions between each of the six or more reactors comprising the second set of catalysts, the varied second set of reaction conditions comprising (i) at least three different space velocities, and (ii) at least two different contact times,

simultaneously discharging a reactor effluent from each of the twelve or more reactors, and

analyzing the reactor effluent from each of the twelve or more reactors to determine the conversion of one or more reactants and the selectivity for one or more products of the chemical reaction of interest in each of the reactors.

46. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values that span at least about 10% conversion difference, and the second set of reaction conditions being varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values that span at least about 10% conversion difference.

47. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values that span at least about 20% conversion difference, and the second set of reaction conditions being varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values that span at least about 20% conversion difference.

48. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 20% to more than about 40%, and the second set of reaction conditions are varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 20% to more than about 40%.

49. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 10% to more than about 50%, and the second set of reaction conditions being varied such that the determined conversion of the conversion-limiting

reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 10% to more than about 50%.

50. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 2% to more than about 5 %, and the second set of reaction conditions being varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 2 % to more than about 5 %.

51. The method of claim 45 wherein the first set of reaction conditions are varied such that a determined conversion of a conversion-limiting reactant for the six or more reactions catalyzed by the first set of catalysts includes a range of six values ranging from less than about 1% to more than about 10 %, and the second set of reaction conditions being varied such that the determined conversion of the conversion-limiting reactant for the six or more reactions catalyzed by the second set of catalysts includes a range of six values ranging from less than about 1 % to more than about 10 %.

52. A method for evaluating process conditions for a catalyzed chemical reaction in a parallel flow reactor, the method comprising

simultaneously supplying one or more reactants to each of sixteen or more reactors of a parallel flow reactor under reaction conditions to effect a chemical reaction of interest, each of the sixteen or more reactors comprising a catalyst having activity for the chemical reaction, the sixteen or more reactors comprising a first set of four or more of the catalysts having substantially the same first composition, a second set of four or more of the catalysts having substantially the same second composition, a third set of four or more of the catalysts having substantially the same third composition, and a fourth set of four or more of the catalysts having substantially the same fourth composition, each of the first composition, the second composition, the third composition and the fourth composition being different from each other,

controllably varying a set of reaction conditions between each of the sixteen or more reactors, the varied set of reaction conditions comprising (i) at least four different

space velocities or contact times or combinations thereof, and (ii) at least four different temperatures, pressures or feed compositions, the set of reaction conditions being varied such that at least one catalyst from each of the first, second, third and fourth sets of catalysts catalyzes the chemical reaction under each of the at least four different space velocities or contact times or combinations thereof, and under each of the at least four different temperatures, pressures or feed compositions,

simultaneously discharging a reactor effluent from each of the sixteen or more reactors, and

analyzing the reactor effluent from each of the sixteen or more reactors to determine the conversion of one or more reactants and the selectivity for one or more products of the chemical reaction of interest in each of the reactors.

53. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of catalysts, includes a range of six values that span at least about 10% conversion difference.

54. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of catalysts, includes a range of six values that span at least about 20% conversion difference.

55. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of

catalysts, includes a range of six values that span at least about 40% conversion difference.

56. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of catalysts, includes a range of six values ranging from less than about 20% to more than about 40%.

57. The method of claim 56 wherein range of six values ranges from less than about 10% to more than about 50%.

58. The method of claim 56 wherein range of six values ranges from less than about 10% to more than about 70%.

59. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of catalysts, includes a range of six values ranging from less than about 2% to more than about 5 %.

60. The method of claim 52 wherein the set of reaction conditions is varied such that a determined conversion of a conversion-limiting reactant for each of (a) the four or more reactions catalyzed by the first set of catalysts, (b) the four or more reactions catalyzed by the second set of catalysts, (c) the four or more reactions catalyzed by the third set of catalysts, and (d) the four or more reactions catalyzed by the forth set of catalysts, includes a range of six values ranging from less than about 1 % to more than about 10 %.

61. The method of claim 52 wherein one or more reactants are simultaneously supplied to each of twenty or more reactors of a parallel flow reactor to effect the chemical reaction of interest, each of the twenty or more reactors comprises a catalyst having activity for the chemical reaction, and four or more of the reactors comprise a reference set of four or more reference catalysts having substantially the same reference composition, each of the four or more reference catalysts catalyzing the chemical reaction under reaction conditions that correspond to four or more of the controllably varied reaction conditions.

62. The method of claim 61 further comprising, for at least one of the first, second, third or fourth catalyst compositions, interpolating or extrapolating at least a portion of a master curve for the reaction of interest defined by a plot of the determined selectivity versus the determined conversion of the reaction of interest for the at least one catalyst composition.

63. The method of claim 62 wherein at least a portion of the master curve is interpolated or extrapolated by comparison with a master curve for the eight or more reference catalysts.

64. The method of claim 52 wherein one or more reactants are simultaneously supplied to each of twenty or more reactors of a parallel flow reactor to effect the chemical reaction of interest, at least sixteen or more reactors comprises a catalyst having activity for the chemical reaction, and at least two or more of the reactors are blank reactors having an essential absence of catalysts having activity for the reaction of interest.

65. The method of claim 52 wherein the reactor effluent from each of the twelve or more reactors are simultaneously analyzed.

66. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different temperatures.

67. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different pressures.

68. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different space velocities, and (ii) at least two different feed compositions.

69. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different temperatures.

70. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different pressures.

71. The method of claim 52 wherein the varied set of reaction conditions comprises (i) at least three different contact times, and (ii) at least two different feed compositions.

72. The method of claim 52 wherein one or more reactants are simultaneously supplied to each of twenty-four or more reactors of a parallel flow reactor to effect the chemical reaction of interest, each of the twenty-four or more reactors comprises a catalyst having activity for the chemical reaction, and the varied set of reaction conditions comprise (i) at least six different space velocities or contact times or combinations thereof, and (ii) at least four different temperatures, pressures or feed compositions, the set of reaction conditions being varied such that at least one catalyst from each of the first, second, third and fourth sets of catalysts catalyzes the chemical reaction under each of the at least six different space velocities or contact times or combinations thereof, and under each of the at least four different temperatures, pressures or feed compositions.